

Innovations through Computational Sciences

NSF-EPS 0556308 (2006-2009)

Mississippi EPSCoR

**Jackson State University, Mississippi State
University, the University of Mississippi,
the University of Southern Mississippi**

Mississippi EPSCoR

- Joint project of the Mississippi Research Consortium (MRC)
 - Jackson State University (JSU)
 - Mississippi State University (MSU)
 - University of Mississippi (UM)
 - University of Southern Mississippi (USM)
- P.I. : Dr. Sandra H. Harpole, Associate Vice President for Research, MSU

Mississippi EPSCoR

- First funded in 1989
- Goal to build research infrastructure
- Significant increases in
 - Proposal submissions (1,327 to a total of 31,954)
 - Awards (799 to a total of 28,207)
 - Publications
 - Collaborations

Innovations through Computational Sciences

- **Goal:**
 - **To establish a national prominence in the computational sciences by enhancing research capacity in the theme area of computational sciences building on the existing strengths in high performance computing**

Innovations through Computational Sciences

- **Theme Areas**
 - **Computational Biology – JSU, MSU, USM**
 - **Computational Chemistry – JSU, UM, USM**
 - **Multi-Scale Biosystem Simulation and Modeling – JSU, MSU, UMMC**
- **Education and Outreach**
- **Evaluation**

Innovations through Computational Sciences

- **Specific Goals:**
 - **Building a national prominence in the theme area of computational sciences**
 - **Increasing research capacity resulting in national competitiveness**
 - **Recruitment of outstanding new faculty with competitive "start-up packages"**

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Specific Goals:

- **Increasing research capacity resulting in national competitiveness**
 - **Support and mentoring of new and existing faculty in interdisciplinary computational sciences research**
 - **Recruitment of excellent graduate students**
 - **Enhancement of computational science infrastructure**

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- **Specific Goals:**
 - **Expanding collaboration among MRC institutions and with outside laboratories**
 - **Growing the pipeline in science, technology, engineering and mathematics (STEM) by**
 - **Expanding opportunities for women and underrepresented groups in the computational sciences**
 - **Increasing the number of graduate students**
 - **Interfacing with K-12 teachers and students.**

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- **Specific Goals:**
 - **Fostering the economic development of the state and nation through development of intellectual property in the computational science area and its commercialization to new spin-off or to partner companies.**

Computational Biology

- Increase number of faculty and staff with expertise in both computational and biological disciplines
 - Recruit five new computational biology faculty
 - Establish graduate research fellowships and seed grants in computational biology
 - Facilitate statewide methods of communication, collaboration and distance learning

Computational Biology

- Scientific focus
 - New techniques in computational biology
 - New paradigms in high performance computing
 - Biological ontology

Computational Biology

- Dr. Susan Bridges-Professor, Computer Science and Engineering (MSU)
- Dr. Shane Burgess-Associate Professor, CVM Basic Science (MSU)
- Dr. Hari H. P. Cohly-(JSU)
- Dr. Raphael D. Isokpehi-(JSU)
- Dr. Frank Moore (USM)

Computational Chemistry

- Cross-disciplinary research to meld computational sciences with experimental data
 - Solvation and Ligand-Biomolecule Interactions
 - Computational Chemistry for Environmental and Industrial Applications
 - Material Chemistry – Metal Complexes, Novel Clusters and Nanoparticles

Computational Chemistry

- Dr. Robert Bateman-Chair & Professor, Chemistry & BioChemistry, (USM)
- Dr. Steven Davis-Professor of Chemistry and Biochemistry, (UM)
- Dr. Glake Hill (JSU)
- Dr. Jerzy Leszczynski (JSU)

Multi-Scale Biosystem Simulation and Modeling

- Biosystem simulation – technique of describing mathematical approximations & computing solutions to approximations using numerical techniques
 - Refinement of the integrative model of human physiology (UMMC, MSU)
 - Multi-scale simulations of an artificial liver device (MSU, UMMC)

Multi-Scale Biosystem Simulation and Modeling

- Biosystem simulation
 - Fluid dynamics of lung respiration and meso-scale aerosol deposition (MSU, JSU, UMMC)

Multi-Scale Biosystem Simulation and Modeling

- Dr. Shahrouz Aliabadi-(JSU)
- Dr. Greg Burgreen, Associate Research Professor, Computational Simulation & Design, MSU
- Dr. Robert Hester, Professor Physiology and Biophysics, UM Medical Center
- Dr. David Marcum, Director, SIM Center, MSU

Education and Outreach

- Common themes
 - Introduce students to inquiry and team-based interdisciplinary research
 - Inform students about careers in computational science
 - Provide students with the support, encouragement and tools needed to continue in related discipline

Education and Outreach

- Educational product development
 - Curricular paths
 - Interdisciplinary courses
 - Computational biology/chemistry/modeling modules

Education and Outreach

- High school juniors/seniors
 - Computational science laboratory experience
 - Mississippi EPSCoR scholarship
- High school teachers/counselors
 - Research and career awareness workshop

Education and Outreach

- Undergraduate students
 - High school recruitment
 - Academic preparation and involvement in a learning community
 - Undergraduate research
 - Statewide networking symposium for undergraduate researchers and mentors

Education and Outreach

- Pamala Heard (JSU)
- Dr. Sherry Herron, Assistant Professor/Director of Science and Math Education, USM
- Dr. Peter Sukanek-Chair and Professor of Chemical Engineering, UM
- Dr. Giselle Thibaudeau-Associate Professor/Director Electron Microscopy, MSU

Evaluation and Assessment

- Evaluation team from JSU, MSU, UM and USM
 - Ms. Georgia Hackney, Research Associate I, Center for Science, Mathematics & Technology, MSU
 - Dr. Sherry Herron, Assistant Professor/Director of Science and Math Education, USM
 - Dr. Amy Wells, Associate Professor of Leadership and Counselor Education, UM
 - Dr. Gregory Opara-Nadi, Program Evaluation Specialist, JSU